INL/CON-08-14877
PREPRINT

Improved Prediction of the Doppler Effect in TRISO Fuel

2009 International Conference on Advances in Mathematics, Computational Methods, and Reactor Physics

J. Ortensi
A. M. Ougouag

May 2009

The INL is a
U.S. Department of Energy
National Laboratory
operated by
Battelle Energy Alliance

International Conference on Mathematics, Computational Methods & Reactor Physics (M&C 2009)
Saratoga Springs, New York, May 3-7, 2009, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2009)

IMPROVED PREDICTION OF THE DOPPLER EFFECT IN TRISO FUEL

J. Ortensi and A. M. Ougouag
Idaho National Laboratory
MS-3870, PO Box 1625, Idaho Falls, ID 83415-3870
Idaho Falls, ID 83415

ABSTRACT

The Doppler feedback mechanism is a major contributor to the passive safety of gas-cooled, graphite-moderated high temperature reactors that use fuel based on Tristructural-Isotropic coated particles. It follows that the correct prediction of the magnitude and time-dependence of this feedback effect is essential to the conduct of safety analyses for these reactors. We present a fuel conduction model for obtaining better estimates of the temperature feedback during moderate and fast transients. The fuel model has been incorporated in the CYNOD-THERMIX-KONVEK suite of coupled codes as a single TRISO particle within each calculation cell. The heat generation rate is scaled down from the neutronic solution and a Dirichlet boundary condition is imposed as the bulk graphite temperature from the thermal-hydraulic solution. This simplified approach yields similar results to those obtained with more complex methods, requiring multi-TRISO calculations within one control volume, but with much less computational effort. We provide an analysis of the hypothetical total control ejection event in the PBMR-400 design that clearly depicts the improvement in the predictions of the fuel temperature. In addition, we have included a brief study of the potential effects of particle layer de-bonding on the transient behavior of high temperature reactors. Although the formation of a gap occurs under special conditions its consequences on the dynamic behavior of the reactor should be analyzed. We show that the presence of a gap in the fuel can cause some unusual reactor behavior during fast transients, but still the reactor shuts down due to the strong Doppler feedback.

Key Words: TRISO, particle, fuel, conduction

1. INTRODUCTION

In High Temperature Reactors (HTRs), the fuel temperature is the principal negative feedback mechanism that allows their safe operation. Modern designs of HTR cores are fueled with Tristructural-Isotropic (TRISO) coated particles. These particles are composed of various layers acting in concert to provide a containment structure that prevents radioactive product release. For a pebble bed reactor (PBR), the TRISO particles are imbedded in a graphite matrix to form a pebble. The same particles are also used in the prismatic design by forming fuel compacts in a cylindrical graphite matrix. The heat transfer characteristics of these components determine the amount of temperature feedback that the reactor will experience. Therefore, any modeling improvements of the heat transfer models result in a better estimate of the Doppler feedback.

A variety of fuel temperature models exist for LWR's that treat the geometry exactly. Some HTGR codes, like THERMIX, only include a pebble or compact shell model, which approximate the temperature of the pebble fuel region. These models produce reasonable results for steady

state and very slow transient conditions. For moderate and fast transients, an explicit model is necessary in order to accurately predict the fuel temperature. These explicit models are also useful to study the heat transfer characteristics at the TRISO level. An approximation to the explicit fuel model is included in the German code TINTE and has been used in the PBMR-400 benchmark exercises [1]. Very recent changes to TINTE allow an improved calculation of the fuel temperature using a multi-TRISO fuel model [2]. The SIEMENS INTERATOM code ZKIND [3] also appears to contain a TRISO level model, but no details are available at this time. In addition, current efforts are focused on explicit TRISO heat transfer via multi-scale models of the PBR and prismatic fuel [4, 5], but it will take some time before they can be used in fully coupled calculations.

2. HEAT CONDUCTION IN TRISO FUEL

From a heat transfer perspective the layered composition of the TRISO generates a natural resistance to heat flow, mainly because of the different thermo-physical properties of the constituent layers. This resistance to heat flow forces the fuel kernels to reach higher temperatures, which rapidly compensate for reactivity insertions. This effect was previously openly identified in 1963 by General Atomics (GA) researchers [6], but the explicit modeling of the fuel particles was never pursued by GA, as far as the authors know, due to the lack of data for the heat transfer model.

2.1. Physical Description of the TRISO Particle and the Formation of a Gap

Tristructural-Isotropic (TRISO) coated particle is composed of a set of functional layers: fuel kernel, porous carbon layer, inner pyrolitic carbon (IPyC), SiC, and outer pyrolitic carbon (OPyC). The main functions of the various layers are heat generation in the kernel, fission product retention in the porous layer, structural integrity in both pyrolitic carbons, and fission product barrier in the SiC.

The various materials that constitute TRISO particles have different thermo-physical and thermo-mechanical properties with varied dynamic behavior. A specific case, further developed in this work, is the formation of a gap via irradiation-induced shrinkage between the buffer and the IPyC. This phenomenon has been observed in some samples of current irradiation programs [7]. It is yet unclear if this effect is magnified by the higher dose rate that the samples experience during accelerated irradiation, but the constituent layers exhibit very different irradiation responses and detach. Nevertheless, the formation of a gap that fills with fission gases and CO, for oxide fuels, can have a significant impact. The fuel performance codes PARFUME and STRESS3 model the layer detachment [8, 9]. Results from these codes indicate that, under the circumstances analyzed, a gap quickly forms during irradiation and remains near a value of 20 μm at fluence levels between $1x10^{25}$ and $4x10^{25}$ n/m^2 [7].

The presence of a gap magnifies the resistance to heat flow out of the fuel region. Essentially, the gap forms a semi-adiabatic system within the TRISO particle, which translates into higher fuel temperatures and, consequently, increased Doppler feedback effects.

2.2. Model Description

The improved approach developed herein incorporates an explicit TRISO heat conduction model to better quantify the temperature in the various layers of the TRISO particle, including its fuel central zone. Figure 1 shows the materials and dimensions used in the model.

Since, physically, the IPyC is not completely detached from the porous carbon layer, some contact area does remain. The size of this contact area varies among TRISO particles and their irradiation history. A set of steady state HEATING 7.3 [10] cases in 3-D spherical geometry were used to determine multipliers for the effective gap conductivity at various heat rates. The carbon density was adjusted in this calculation to maintain mass conservation. These multipliers are used to increase the conductivity in the gap region by correcting the full (4π steradiant) gap model.

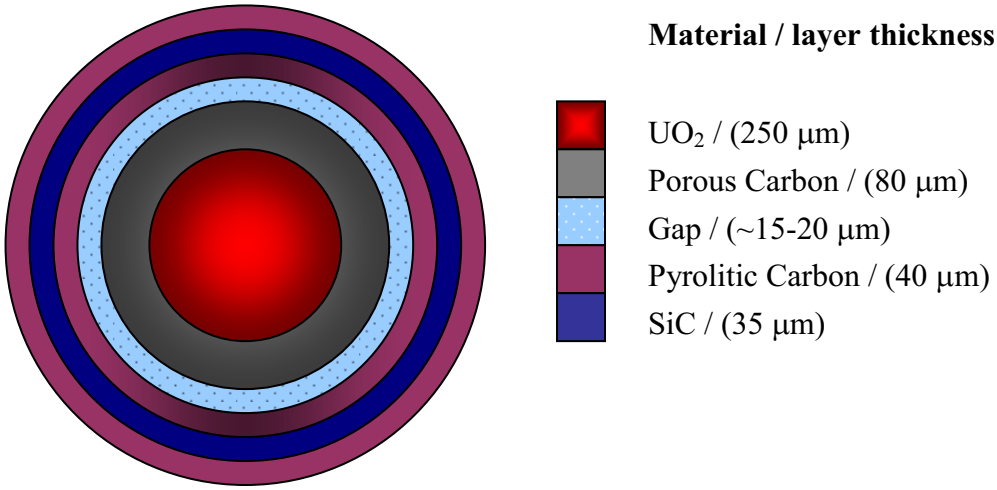

Figure 1. TRISO model composition

Consider the 1-D spherical heat flux formulation of the heat conduction equation

$$-\nabla\cdot\vec{q}(r,t)+q'''_{tr}(r,t)=\frac{\partial}{\partial t}\left[\rho(r,t)C_p(r,t)T(r,t)\right] \qquad 0\le r\le R \quad \text{for } t\ge 0 \qquad (1)$$

A Neumann condition is imposed at the center and a Dirichlet condition at the outer boundary

$$\left.\frac{\partial T(r,t)}{\partial r}\right|_{r=0} = 0 \qquad \text{T(R)=T}_{\text{graphite}} \qquad \text{for t > 0} \qquad (2)$$

The balance equation is obtained by integrating Eq. 1 over the volume of the cell. Introducing the time discretization scheme leads to:

$$-A_{i+1}\vec{q}_i(r_{i+1},t)\cdot\hat{n}_{i+1} + A_i\vec{q}_i(r_i,t)\cdot\hat{n}_i + q_i'''V_i = \widetilde{C}_i\left(\frac{\widetilde{T}_i^{n+1}-\widetilde{T}_i^{n}}{t^{n+1}-t^{n}}\right) \qquad (3)$$

Where $\widetilde{C}_i$ is the effective heat capacity.

Using Fourier's law as the closure model in Eq. (3) and forcing the continuity of the heat flux at the interfaces yields a three point formulation with the average cell temperatures. With the introduction of a theta differencing scheme we arrive to the equation:

$$\theta\left(a_{i+1}\widetilde{T}_{i+1}^{n+1} + a_i\widetilde{T}_i^{n+1} + a_{i-1}\widetilde{T}_{i-1}^{n+1}\right) = \left((1-\theta)q_i'''^{n} + \theta q_i'''^{n+1}\right)V_i + (1-\theta)\left(b_{i+1}\widetilde{T}_{i+1}^{n} + b_i\widetilde{T}_i^{n} + b_{i-1}\widetilde{T}_{i-1}^{n}\right) \qquad (4)$$

Since the final matrix is positive definite, tri-diagonal, and symmetric, the direct inversion of the two banded system of equations yields the final solution.

2.3. Material Properties

The conductivities and specific heat capacities incorporated in this preliminary model are depicted in Figures 2 and 3, respectively. The calculation of the actual gap conductivity is based on the RELAP5-3D© non-condensable gas model [11].

These material libraries are currently under review to ensure the thermo-physical properties are representative of the latest TRISO designs and fuel performance programs.

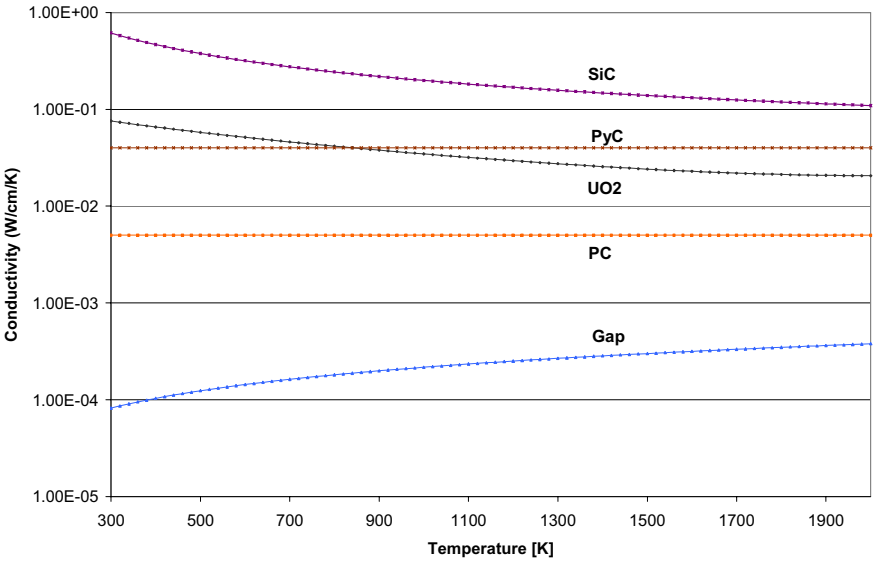

Figure 2. Thermal conductivities for the TRISO constituent layers

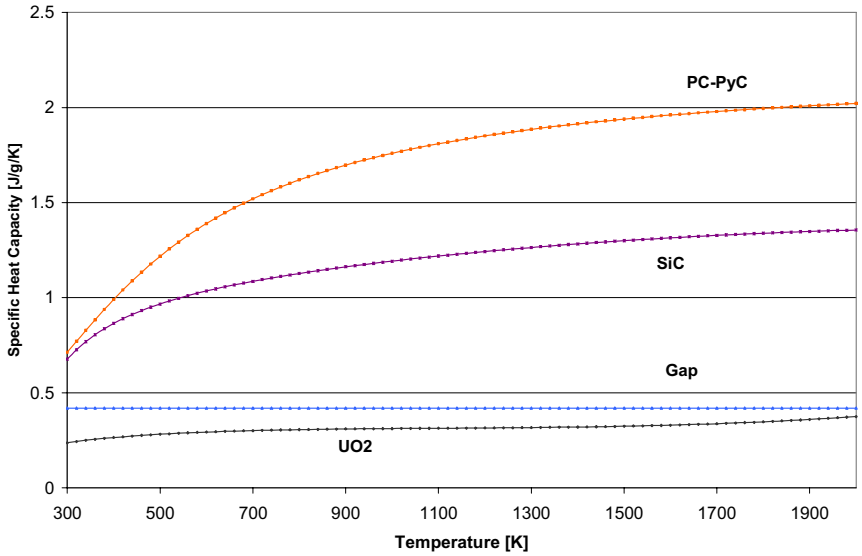

Figure 3. Specific heat capacities for the TRISO constituent layers

3. INCORPORATION INTO THE COUPLED CODE

The 1-D Finite Volume TRISO model was incorporated into the CYNOD-THERMIX-KONVEK suite. CYNOD [12] is a semi-analytical nodal diffusion code based on a Green's function method with an implicit time dependent scheme. CYNOD is coupled to the thermal-hydraulics code THERMIX-KONVEK [13], a two-dimensional (R-Z) quasi-static code developed by the KFA-Jülich, which contains correlations and material properties developed in the German PBR program.

The TRISO model is applied within each calculation cell and uses the cell averaged power density, renormalized to the kernel volume, as the heat generation source. The bulk graphite temperature from the thermal hydraulics calculation is used as the boundary condition at the OPyC-matrix interface. The main idea behind this simplified modeling is to capture the behavior of the average TRISO particle in each calculation cell in a manner that is easily implemented in the current suite of codes to provide some preliminary capability for analysis. The use of the Dirichlet condition with the bulk graphite temperature allows for a fast coupling of the heat transfer models to obtain a representative fuel temperature.

The total control rod ejection (TCRE) problem from the PBMR benchmark exercise was used to examine the potential benefits of the new method. This is an unrealistic transient but it serves to determine the capabilities of the new explicit TRISO model in extreme cases. Three different fuel temperature calculation methods were used in the analysis: a quasi- static homogenous shell model from THERMIX (QSHo), a quasi-static heterogeneous TRISO model (QSHe), and the time dependent heterogeneous TRISO model (TDHe).

An additional set of calculations used the heterogeneous TRISO models in the presence of a gap with gap sizes up to 20 μm and geometric configurations with contact regions determined by polar angles of $\pi/4$, $\pi/2$ and $3\pi/4$ steradiants.

4. NUMERICAL RESULTS

4.1 Benchmarking of the TRISO Model

The stand alone TRISO code was benchmarked against the analytic solution to the 1D spherical time-dependent conduction equation with homogeneous, constant thermo-physical properties and various heat generation rates (fixed, linear, exponential). In addition, the code was compared to the finite difference code HEATING 7.3 to check the results of the multi-layer model with variable thermo-physical properties. Figure 5 shows the percent error in the temperature calculations in both codes when compared to the analytic solution. The small differences seen in HEATING 7.3 appear to arise from the solution methodology.

Figure 6 presents a comparison to the HEATING 7.3 results obtained for a model with variable properties in all of the layers and for an assumed power excursion. The code-to-code comparisons show good agreement with maximum differences of 0.06%.

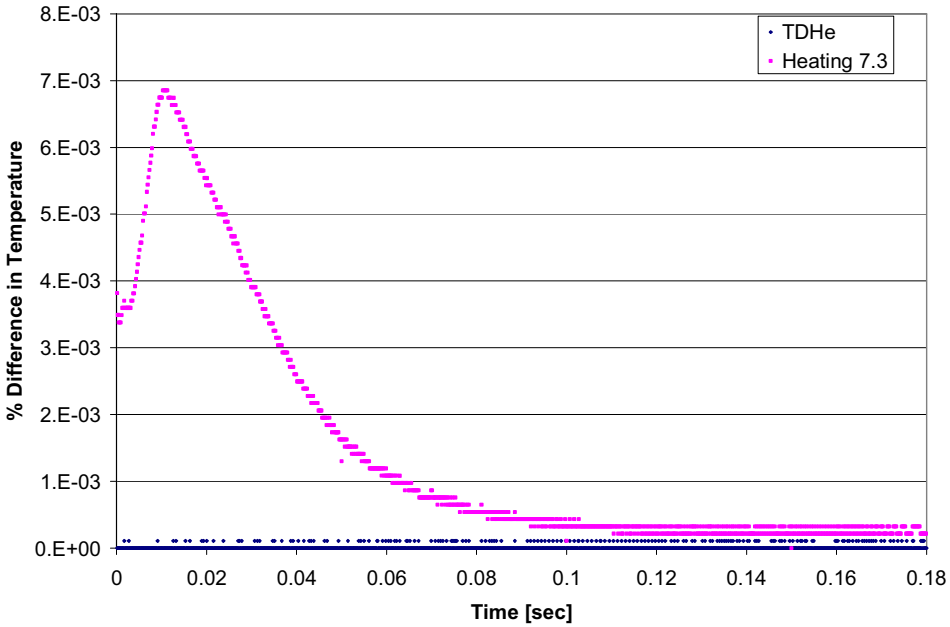

Figure 5. Comparison to the analytic solution of a 1D homogeneous sphere with exponential heat generation and fixed thermo-physical properties

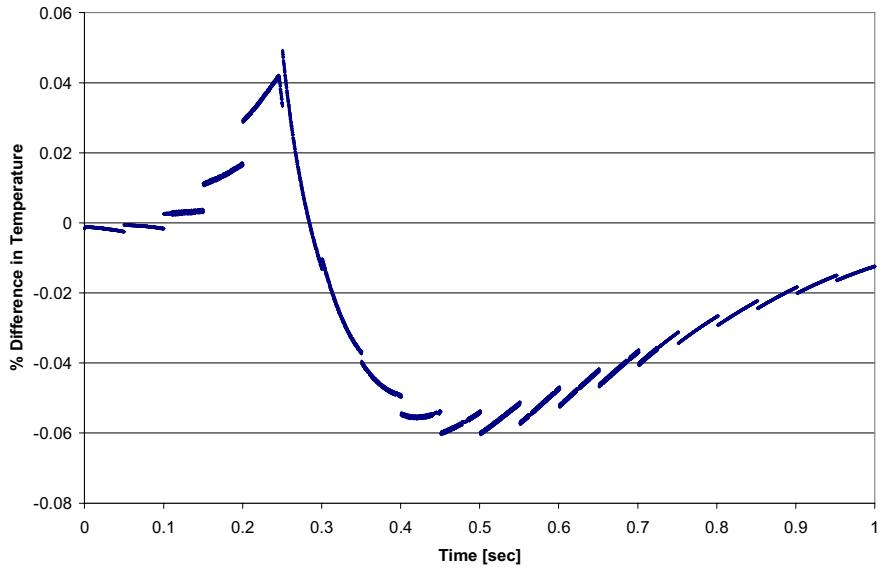

Figure 6. Code-to-code comparison for the multilayered model with variable heat generation and variable thermo-physical properties.

4.2 Fast Transient Analysis Results without the TRISO Gap

The results obtained with the homogeneous and the TRISO level models in CYNOD-THERMIX are displayed in Figure 7. The results confirm the considerable improvement over the predictions of the homogeneous model. The incorporation of the enhanced model shows that the Doppler Effect plays a more significant role than predicted by the original unenhanced model based on the THERMIX homogenized fuel region. The calculated maximum powers attained with the QSHo, QSHe, and TDHe methods are roughly 160, 26, and 30 times the nominal power. Therefore the QSHo model overestimates the reactor power by a factor of 130 and the QSHe underestimates the reactor power by a factor of 4.

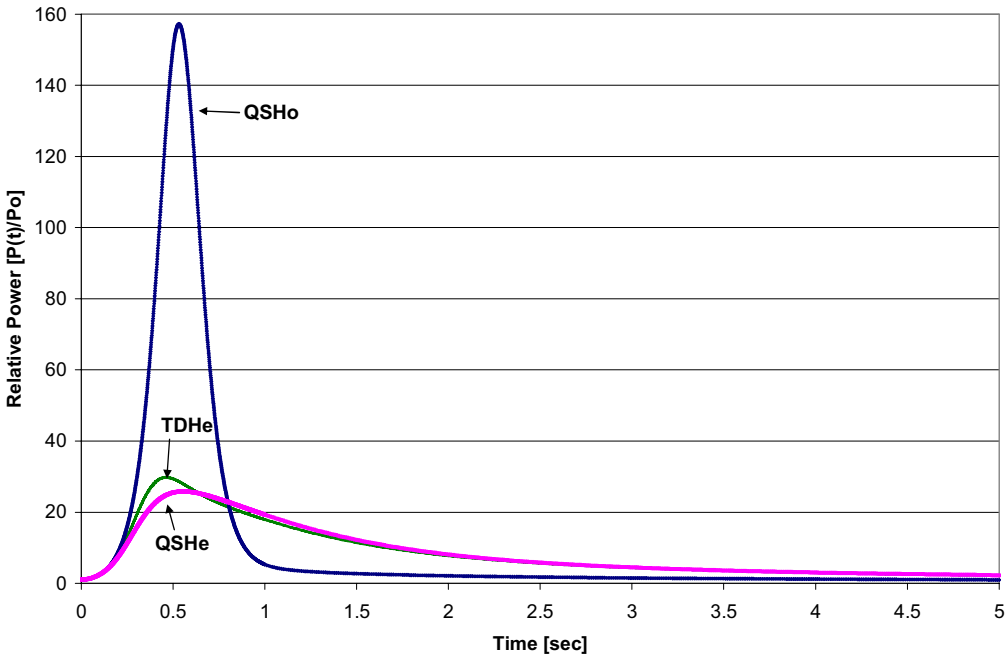

Figure 7. Comparison of the relative core power during a TCRE with three different fuel models

In comparison to the TINTE results [14], the maximum fission power calculated by the TDHe model is 11904 MW and agrees well with the value of 11750 MW from TINTE. The maximum fuel temperatures in the core are 1700 ^{o}C and 1768 ^{o}C with the TDHe model and TINTE, respectively. The power decrease is sharper in our model as well. These differences are probably due to the fact that we are using variable thermo-physical properties. The new model also reveals that the overall energy generation during the rod ejection transient is 12% lower than predicted by the unenhanced model. In addition, the power behavior obtained with the enhanced model indicates that the reactor period during the cool down is longer than previously predicted with the homogenous fuel region model. Figure 8 shows that the average fuel temperature in the core reaches a slightly higher maximum, but at no time does it approach the nominal, allowable TRISO fuel temperature of 1600 ^{o}C.

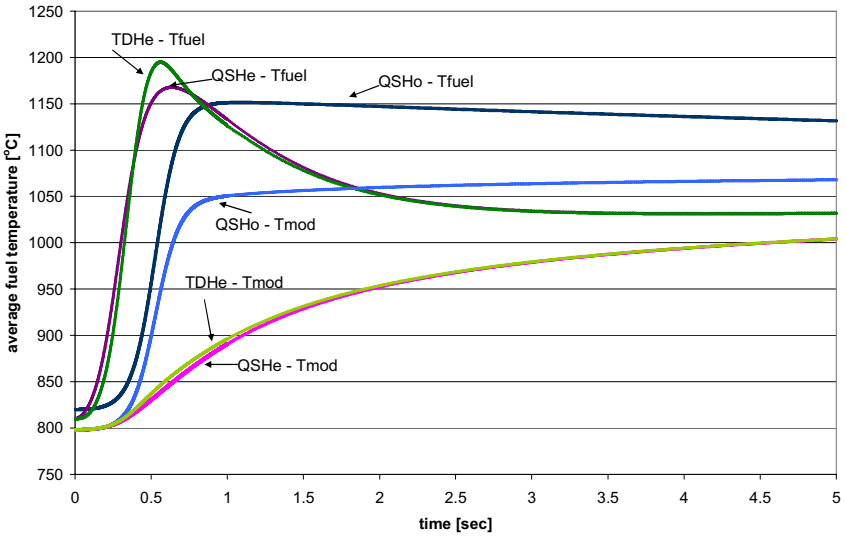

Figure 8. Comparison of the fuel and moderator temperatures during a TCRE

4.3 Fast Transient Analysis Results with the TRISO Gap

Figure 9 shows a set of calculations with the QSHe model with a 4π steradiant gap. The gap size ranges from a closed gap to a 20 micron gap. The core power profile decreases in amplitude with an increasing gap size. The relative power drops by an additional factor of 20 with the 20 micron gap and the period of the reactor also increases with increasing gap size. The amount of energy generation during the rod ejection transient decreases with the enhanced calculation of the Doppler feedback since the area under the curve is reduced.

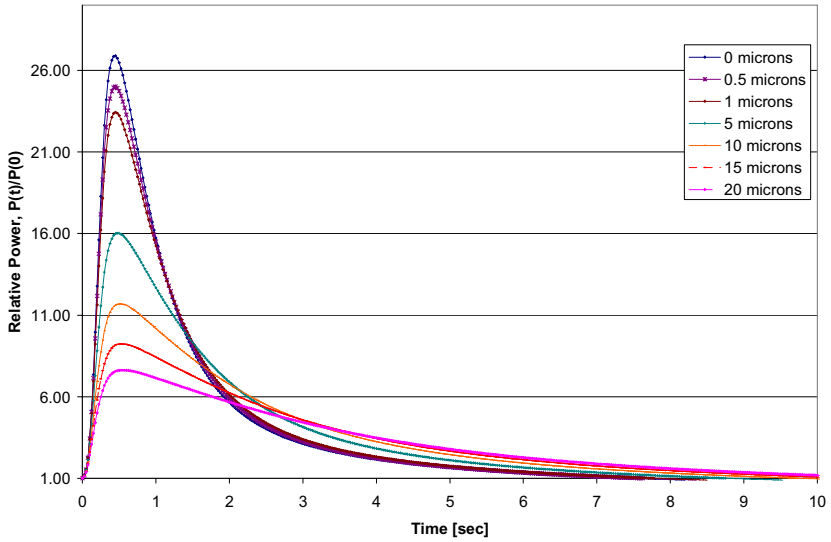

Figure 9. Effects of a TRISO gap on the relative core power with the quasi-static heterogeneous model

Figures 11 and 12 show the preliminary results for the core power and temperature profiles of the TCRE using the TDHe model with a 20μm gap. The plot also includes an eigenvalue calculation during the transient. There is a dramatic difference between the quasi-static and the time-dependent models, since the QSHe is unable to capture the dynamic effects that take place in the TRISO particle. The relatively small conductivity of the gap establishes a large resistance to heat flow and results in higher fuel temperatures. These higher fuel temperatures and the consequent Doppler feedback place the reactor into a sub-critical condition within 0.4 seconds of the start of the transient.

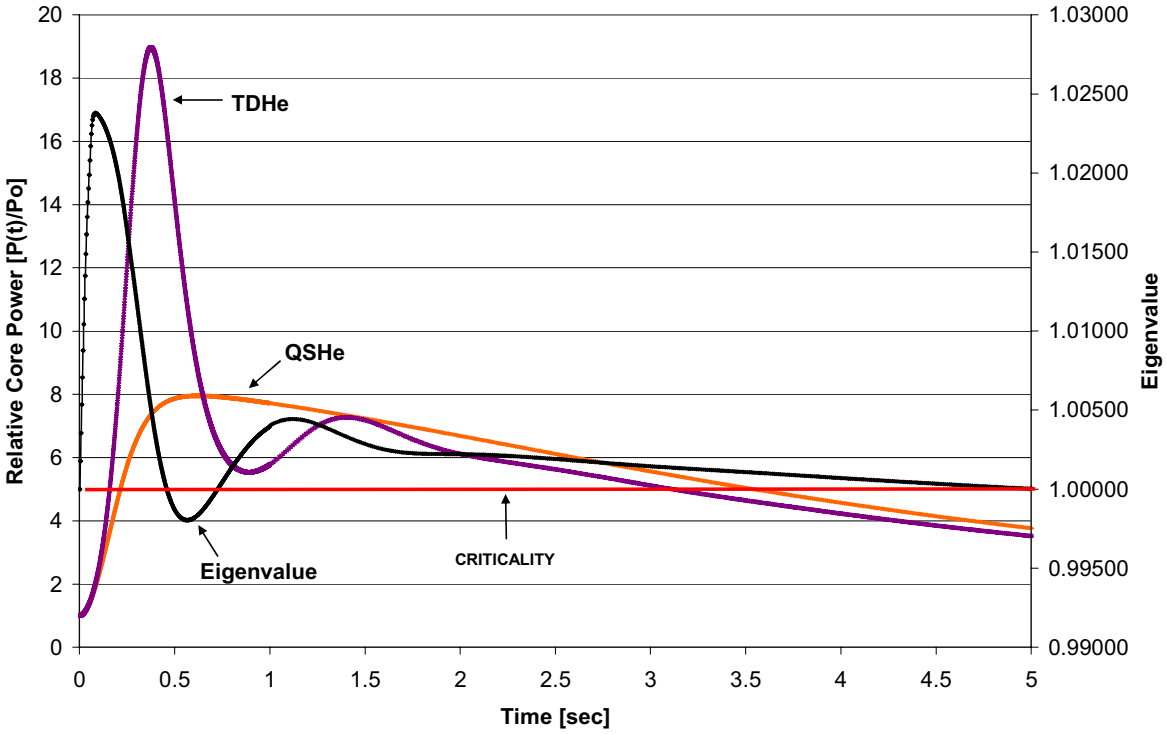

Figure 11. Relative core power during a TCRE with a TRISO gap

In addition, as the fuel temperature increases the UO_2 thermal conductivity decreases and its heat capacity increases, thus creating an energy storage or "capacitor" effect. This heat is subsequently released when the gap conductivity increases with temperature, thus allowing better heat transfer out of the kernel. The improved heat transfer and the rapid decrease in heat generation facilitate the fast cool down of the kernel, which in turn decrease resonance capture. This allows the neutron population to increase again as the reactor returns to a delayed-supercritical condition for approximately 4 seconds. These results are preliminary since there is a slight mismatch in the time scale of the solution. The relative power starts to turn at 0.38 seconds, but the sub-critical configuration is not attained until 0.46 seconds. The opposite is true for the next power escalation where the delayed-super-critical condition is reached at 0.76 sec and the power turns at 0.9 sec.

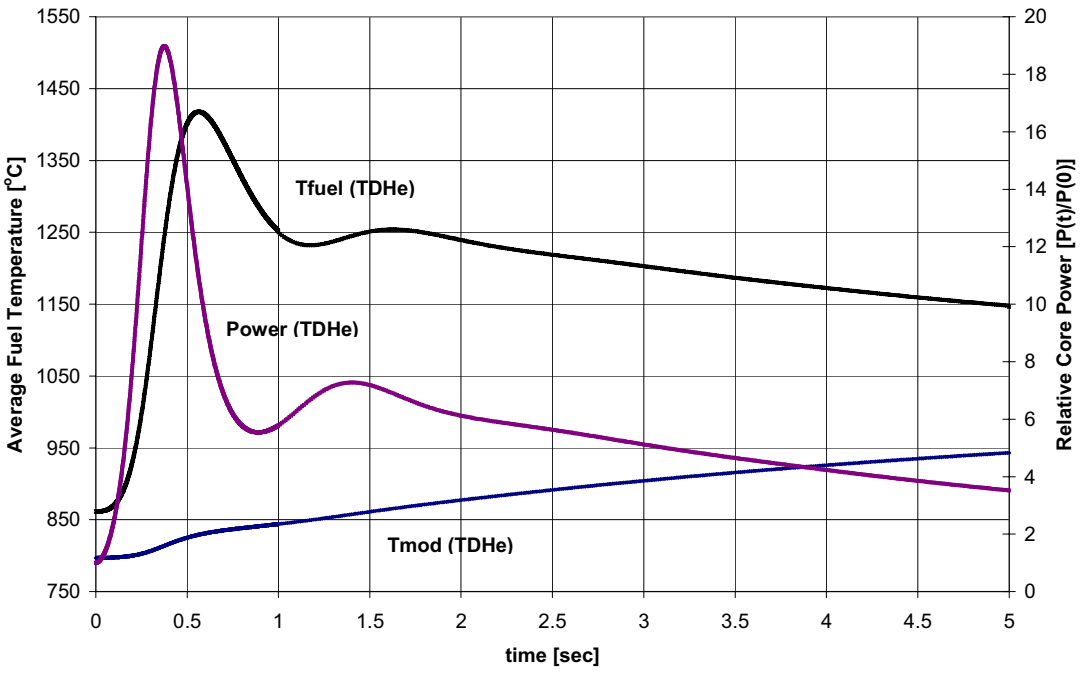

Figure 12. Average fuel and moderator temperatures during a TCRE with a TRISO gap

4.4 Gap Conductivity Multipliers

Table I shows the results from the HEATING 7.3 3-D calculations used to determine the gap conductivity multipliers to correct the 4π steradiant gap model for the presence of a contact area.

Table I. Conductivity correction factors

Heat Rate [W]	θ=π/4 A=14.64%	θ=π/2 A=50%	θ=3π/4 A=85.36%
0.144	1.436	2.786	5.021
0.311	1.448	2.713	4.892
0.543	1.423	2.637	4.690
0.699	1.416	2.606	4.608

Figure 13 shows the results obtained with the various corrections to the gap conductivities from Table I. As the gap closes the core power profile approaches the behavior of the fuel without the gap, where the fluctuation between subcritical and delayed super-critical state is avoided. The π/4 sr case shows a different core power behavior than the other runs, which seems to indicate the presence of a transition point or that the functionalization of the conductivity in table I is not sufficient to capture the effect correctly.

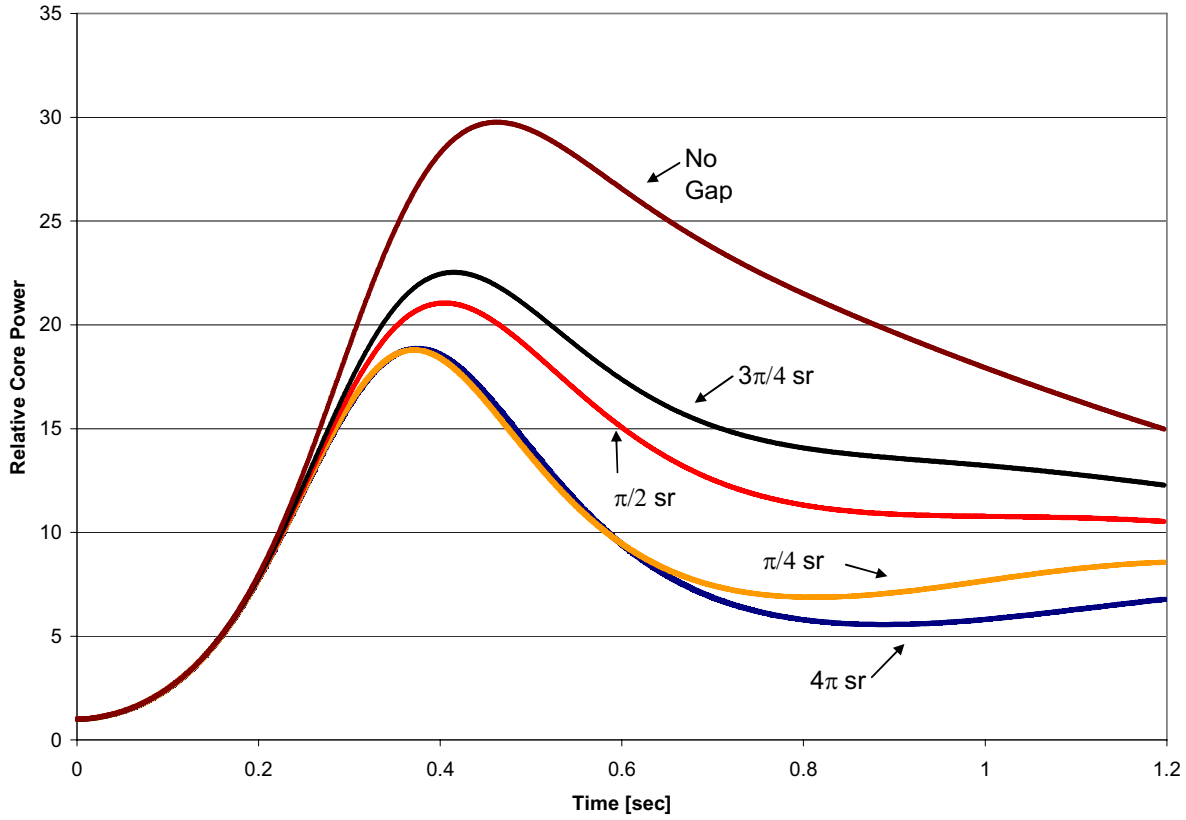

Figure 13. Relative core powers with variable contact areas between the IPYC and porous carbon layers

3. CONCLUSIONS

A simple and efficient way of calculating fuel temperature in TRISO fueled reactors has been presented. The model was benchmarked against analytic solutions and it performed well in code-to-code comparison with Heating 7.3. The results show that both the quasi-static and the time-dependent heterogeneous models are a great improvement over the homogenous model for the study of the HTGR core behavior during fast transient. We have shown that a time-dependent heterogeneous model is able to capture dynamic effects that the quasi-static heterogeneous model is unable to capture. The fuel temperature calculations performed with the CYNOD-THERMIX-KONVEK suite are comparable to those of TINTE. We also show that the presence of a gap in all or most TRISO fuel can change the dynamic behavior of the reactor. The gap creates a "thermal resistor" effect in the TRISO, where energy is stored until the proper conditions enable the release of energy.

ACKNOWLEDGMENTS

Work supported by the U.S. Department of Energy, Assistant Secretary for the office of Nuclear Energy, under DOE Idaho Operations Office Contract DE-AC07-05ID14517.

REFERENCES

1. "OECD/NEA/NSC PBMR Coupled Neutronic/Thermal Hydraulics Transient Benchmark: The PBMR-400 Core Design," Draft 07 (2007).
2. O. Ubbink, et al., "PBMR Fuel Kernel Model for the Prediction of Accurate Temperature Profiles," ICONE16, Orlando, FL, USA, May 11-15 (2008).
3. T. Rademer, W. Bernnat, G. Lohnert, "Coupling of Neutronics and Thermal-Hydraulics Codes for the Simulation of Transients of Pebble Bed HTR Reactors," *High Temperature Reactor Technology*, Beijing, China, September 22-24, (2004).
4. R. Stainsby, et al. "Development of Local Heat Transfer Models for Safety Assessment of the Pebble Bed High Temperature Gas-Cooled Reactor Cores," *High Temperature Reactor Technology*, Washington, USA, September 28 - October 1, (2008).
5. R. Stainsby, et al. "Development of Local Heat Transfer Models for the Safety Assessment of Prismatic Modular High Temperature Gas-Cooled Reactor Cores," *High Temperature Reactor Technology*, Washington, USA, September 28 - October 1, (2008).
6. M.H. Merrill, "Calculation Procedures for Evaluating Transients in Semihomogeneous Power Reactors," Reactor Kinetics and Control, *Atomic Energy Commission Symposium 2* (1963).
7. G.K. Miller, D. L. Knudson. **"**An evaluation of the Gap Between the Buffer and IPyC Layers During Irradiation of a TRISO-Coated Fuel Particle.", INL Engineering Design File 6872. April 2006.
8. G.K. Miller, et al. "Current Capabilities of the Fuel Perforamce Modeling Code Parfume," *High Temperature Reactor Technology*, Beijing, China, September 22-24, (2004).
9. D.G. Martin, "The Mathematical Basis of STRESS3 and STAPLE, HTR-F WP3/DGM/03/04," November 2003.
10. K.W. Childs, PSR-0199/05, HEATING 7.3 (2007).
11. "RELAP5-3D© Manuals, Volume 4: Models and Correlations," INEEL-EXT-98-00834-V1,06/2005.
12. H. Hiruta, et al. "CYNOD: a Neutronics Code for Pebble Bed Modular Reactor Coupled Transient Analysis. HTR (2008).
13. E. Teuchert et al, "V.S.O.P.('94) Computer Code System for Reactor Physics and Fuel Cycle Simulation - Input Manual and Comments." April 1994.
14. G. Strydom, "TINTE Transient Results for the OECD 400 MW PBMR Benchmark," ICAPP '08, Anheim, CA, USA, June 8-12 (2008).